Decision Trees

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Co-instructor: Ziv Bar-Joseph

Machine Learning 10-701
• Question: What function does a decision tree represent?
  – Recall that in linear regression, we used a linear function of the input to predict the output
Decision Tree for Tax Fraud Detection

- Each internal node: test one feature $X_i$
- Each branch from a node: selects some value for $X_i$
- Each leaf node: prediction for $Y$
Prediction

• Question: Given a decision tree, how do we assign a label to a test point?
Decision Tree for Tax Fraud Detection

Query Data

<table>
<thead>
<tr>
<th>$X_1$</th>
<th>$X_2$</th>
<th>$X_3$</th>
<th>$Y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Refund</td>
<td>Marital Status</td>
<td>Taxable Income</td>
<td>Cheat</td>
</tr>
<tr>
<td>No</td>
<td>Married</td>
<td>80K</td>
<td>?</td>
</tr>
</tbody>
</table>

Refund

- Yes
  - NO
- No
  - MarSt
    - Single, Divorced
    - TaxInc
      - < 80K
        - NO
      - > 80K
        - YES
  - Married
    - NO
Decision Tree for Tax Fraud Detection

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<table>
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<tr>
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Decision Tree for Tax Fraud Detection

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Decision Path:
- Refund: No
- MarSt: Married
- TaxInc: > 80K
  - NO: Yes
  - < 80K: NO
Decision Tree for Tax Fraud Detection

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Refund

NO

MarSt

NO

TaxInc

NO

< 80K

NO

> 80K

YES
Decision Tree for Tax Fraud Detection

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Refund: YES
Refund: NO

MarSt: Single, Divorced
MarSt: Married

TaxInc: < 80K
TaxInc: > 80K

NO
NO
NO
YES
Decision Tree for Tax Fraud Detection

Refund
- Yes
  - NO
- No
  - MarSt
    - Single, Divorced
    - TaxInc
      - < 80K
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Assign Cheat to “No”
So far...

• What function does a decision tree represent
• Given a decision tree, how do we assign label to a test point

Now ...

• How do we learn a decision tree from training data?
How to learn a decision tree

- Top-down induction [ID3]

Main loop:
1. $X \leftarrow$ the “best” decision feature for next node
2. Assign $X$ as decision feature for node
3. For each value of $X$, create new descendant of node (Discrete features)
4. Sort training examples to leaf nodes
5. If training examples perfectly classified, Then STOP, Else iterate over new leaf nodes (steps 1-5) after removing current feature

6. When all features exhausted, assign majority label to the leaf node
Which feature is best?

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<td>T</td>
<td>T</td>
<td>T</td>
</tr>
<tr>
<td>T</td>
<td>F</td>
<td>T</td>
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Good split if we are more certain about classification after split – Uniform distribution of labels is bad
Which feature is best?

Pick the attribute/feature which yields maximum information gain:

$$\arg \max_i I(Y, X_i) = \arg \max_i [H(Y) - H(Y | X_i)]$$

$$H(Y)$$ – entropy of Y  \hspace{1cm} $$H(Y | X_i)$$ – conditional entropy of Y
Andrew Moore’s Entropy in a Nutshell

Low Entropy

..the values (locations of soup) sampled entirely from within the soup bowl

High Entropy

..the values (locations of soup) unpredictable... almost uniformly sampled throughout our dining room
Entropy

- Entropy of a random variable $Y$

$$H(Y) = - \sum_y P(Y = y) \log_2 P(Y = y)$$

More uncertainty, more entropy!

$Y \sim \text{Bernoulli}(p)$

Information Theory interpretation: $H(Y)$ is the expected number of bits needed to encode a randomly drawn value of $Y$ (under most efficient code)
Information Gain

• Advantage of attribute = decrease in uncertainty
  – Entropy of Y before split
    \[ H(Y) = - \sum_{y} P(Y = y) \log_2 P(Y = y) \]
  – Entropy of Y after splitting based on \( X_i \)
    • Weight by probability of following each branch
    \[
    H(Y | X_i) = \sum_{x} P(X_i = x) H(Y | X_i = x) \\
    = - \sum_{x} P(X_i = x) \sum_{y} P(Y = y | X_i = x) \log_2 P(Y = y | X_i = x)
    \]

• Information gain is difference
  \[ I(Y, X_i) = H(Y) - H(Y | X_i) \]

Max Information gain = min conditional entropy
Which feature is best to split?

Pick the attribute feature which yields maximum information gain:

$$\arg \max_i I(Y, X_i) = \arg \max_i [H(Y) - H(Y|X_i)]$$

$$= \arg \min_i H(Y|X_i)$$

Entropy of Y

$$H(Y) = - \sum_y P(Y = y) \log_2 P(Y = y)$$

Conditional entropy of Y

$$H(Y | X_i) = \sum_x P(X_i = x) H(Y | X_i = x)$$

Feature which yields maximum reduction in entropy (uncertainty) provides maximum information about Y
### Information Gain

\[
H(Y \mid X_i) = - \sum_x P(X_i = x) \sum_y P(Y = y \mid X_i = x) \log_2 P(Y = y \mid X_i = x)
\]

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<td>F</td>
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<td>F</td>
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<td>F</td>
<td>T</td>
<td>F</td>
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\[
\hat{H}(Y \mid X_1) = -\frac{1}{2}[1\log_2 1 + 0\log_2 0] - \frac{1}{2}[\frac{1}{4}\log_2 \frac{1}{4} + \frac{3}{4}\log_2 \frac{3}{4}]
\]

\[
\hat{H}(Y \mid X_2) = -\frac{1}{2}[-\frac{3}{4}\log_2 \frac{3}{4} + \frac{1}{4}\log_2 \frac{1}{4}] - \frac{1}{2}[\frac{1}{2}\log_2 \frac{1}{2} + \frac{1}{2}\log_2 \frac{1}{2}]
\]

\[
\hat{H}(Y \mid X_1) < \hat{H}(Y \mid X_2)
\]

> 0
How to learn a decision tree

• Top-down induction [ID3]

Main loop:
1. $X \leftarrow$ the “best” decision feature for next node
2. Assign $X$ as decision feature for node
3. For each value of $X$, create new descendant of node (Discrete features)
4. Sort training examples to leaf nodes
5. If training examples perfectly classified, Then STOP, Else iterate over new leaf nodes (steps 1-5) after removing current feature

6. When all features exhausted, assign majority label to the leaf node
How to learn a decision tree

• Top-down induction [ID3, C4.5, C5, ...]

Main loop:  

C4.5

1. \( X \leftarrow \) the “best” decision feature for next node
2. Assign \( X \) as decision feature for node
3. For “best” split of \( X \), create new descendants of node
4. Sort training examples to leaf nodes
5. If training examples perfectly classified, Then STOP, Else iterate over new leaf nodes
6. Prune back tree to reduce overfitting
7. Assign majority label to the leaf node

Refund

MarSt

TaxInc

< 80K

> 80K

Single, Divorced

Married

NO

NO

NO

YES
Handling continuous features (C4.5)

Convert continuous features into discrete by setting a threshold.

What threshold to pick?

Search for best one as per information gain. Infinitely many??

Don’t need to search over more than ~ n (number of training data), e.g. say $X_1$ takes values $x_1^{(1)}$, $x_1^{(2)}$, ..., $x_1^{(n)}$ in the training set. Then possible thresholds are

$$[x_1^{(1)} + x_1^{(2)}]/2, [x_1^{(2)} + x_1^{(3)}]/2, ..., [x_1^{(n-1)} + x_1^{(n)}]/2$$
Dyadic decision trees
(split on mid-points of features)
Decision Tree more generally...

- Features can be discrete, continuous or categorical
- Each internal node: test some set of features \( \{X_i\} \)
- Each branch from a node: selects a set of value for \( \{X_i\} \)
- Each leaf node: prediction for \( Y \)
When to Stop?

• Many strategies for picking simpler trees:
  – Pre-pruning
    • Fixed depth (e.g. ID3)
    • Fixed number of leaves
  – Post-pruning
    • Chi-square test
      – Convert decision tree to a set of rules
      – Eliminate variable values in rules which are independent of label (using chi-square test for independence)
      – Simplify rule set by eliminating unnecessary rules
  – Information Criteria: MDL (Minimum Description Length)
Information Criteria

• Penalize complex models by introducing cost

\[
\hat{f} = \arg \min_T \left\{ \frac{1}{n} \sum_{i=1}^{n} \text{loss}(\hat{f}_T(X_i), Y_i) + \text{pen}(T) \right\}
\]

log likelihood cost

\[
\text{loss}(\hat{f}_T(X_i), Y_i) = (\hat{f}_T(X_i) - Y_i)^2
\]

regression classification

\[
\text{loss}(\hat{f}_T(X_i), Y_i) = 1_{\hat{f}_T(X_i) \neq Y_i}
\]

penalize trees with more leaves

CART – optimization can be solved by dynamic programming
Example of 2-feature decision tree classifier
How to assign label to each leaf

Classification – Majority vote

Regression – ?
How to assign label to each leaf

Classification – Majority vote

Regression – Constant/Linear/Poly fit
Regression trees

\[ X^{(1)} \quad \ldots \quad X^{(p)} \quad Y \]

<table>
<thead>
<tr>
<th>Gender</th>
<th>Rich?</th>
<th>Num. Children</th>
<th># travel per yr.</th>
<th>Age</th>
</tr>
</thead>
<tbody>
<tr>
<td>F</td>
<td>No</td>
<td>2</td>
<td>5</td>
<td>38</td>
</tr>
<tr>
<td>M</td>
<td>No</td>
<td>0</td>
<td>2</td>
<td>25</td>
</tr>
<tr>
<td>M</td>
<td>Yes</td>
<td>1</td>
<td>0</td>
<td>72</td>
</tr>
<tr>
<td>:</td>
<td>:</td>
<td>:</td>
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Average (fit a constant) using training data at the leaves

- Female: Predicted age = 39
- Male: Predicted age = 36
Example of decision tree classifier with dyadic splits (mid-point of feature)
Expressiveness of Decision Trees

- Decision trees in general (without pruning) can express any function of the input features.
- E.g., for Boolean functions, truth table row $\rightarrow$ path to leaf:

\[
\begin{array}{ccc}
A & B & A \text{ xor } B \\
F & F & F \\
F & T & T \\
T & F & T \\
T & T & F \\
\end{array}
\]

\[
\begin{array}{c}
\text{A} \\
\text{B} \\
\text{B} \\
\text{F} \\
\text{T} \\
\text{T} \\
\text{F} \\
\text{T} \\
\text{F} \\
\text{F} \\
\end{array}
\]

- There is a decision tree which perfectly classifies a training set with one path to leaf for each example - overfitting
- But it won't generalize well to new examples - prefer to find more compact decision trees
Decision Trees - Overfitting

One training example per leaf – overfits, need compact/pruned decision tree
What you should know

• Decision trees are one of the most popular data mining tools
  • Interpretability
  • Ease of implementation
  • Good performance in practice (for small dimensions)
• Information gain to select attributes (ID3, C4.5,...)
• Can be used for classification, regression and density estimation too
• Decision trees will overfit!!!
  – Must use tricks to find “simple trees”, e.g.,
    • Pre-Pruning: Fixed depth/Fixed number of leaves
    • Post-Pruning: Chi-square test of independence
    • Complexity Penalized/MDL model selection